Effective dimension of quasiparticle states and remnant Fermi surface in oxychlorides $Ca_2CuO_2Cl_2$ and $Sr_2CuO_2Cl_2$

V.A.Gavrichkov

L.V.Kirensky Institute of Physics

Abstract

Formal similarity between $\overrightarrow{k}-$ area for the contribution from ZR-states and the remnant Fermi surface has been found. Presence of the contribution from $^3B_{1g}-$ states at other $\overrightarrow{k}-$ area means the two-channel processes of scattering. As consequence, the method of integration with a constant energy interval reproduces not only remnant Fermi surface at least , but one of the contributions of above states to the total spectral intensity

101

Contents

Oxychlorides $Ca_2CuO_2Cl_2$ and $Sr_2CuO_2Cl_2$ are antiferromagnetic insulators with Neel temperatures of $255K$ and $247K$, respectively. The spectral intensity in angle resolved photoemission spectroscopy (ARPES) of the oxychlorides gives the information about the nature of a single hole in CuO_2 - plane. Here, we are interested the only the low-energy exitations or so-called first electron-removal states. The spectral intensity of the first electron-removal state in the oxychlorides – amplitude quasiparticle peak (QP) shows a sudden drop along a line in $\vec{k}$ - space which closely resembles the Fermi surface (FS) obtained in the band-structure calculation or ARPES data of the optimally or overdoped high temperature superconductors (HTSCs). Comparing the binding energies of the first electron-removal states at $\vec{k}$ - wave vectors on the remnant FS one can formally define a gap [1]. The gap dispersion of the QP peak along $\vec{k}$ - contour of the remnant FS is close to the d- wave-superconductivity gap in the optimal and overdoped HTSCs, i.e. there is a clear connection between all three energy gaps.

The recent ARPES – experiments for the oxychlorides have shown that there is a strong dependence of the amplitude of QP on a photon energy [2]. For $21eV$ - photon energy there is the clear QP at $\vec{k} = (\pi/2 + \epsilon, \pi/2 + \epsilon)$. And the amplitudes of peak at $\vec{k} = (\pi/2 - \epsilon, \pi/2 - \epsilon)$ and $\vec{k} = (\pi/2 + \epsilon, \pi/2 + \epsilon)$ are approximately equal each other. In really, it is a strange behavior of spectral intensity in a vicinity of the remnant FS where we have the right to expect the asymmetry in the amplitudes of QP at these two $\vec{k}$ - points irrespective of the photon energy. A probable explanation is the matrix element effect in ARPES- data [2]. The later, in turn, points out that there is the different nature of the first electron-removal state at the different $\vec{k}$ - wave vectors. However, according to the generally accepted conclusion, these states have A_{1g} - symmetry of Zhang-Rice (ZR-) state on all BZ. This statement is coordinated with the polarized ARPES – data [3]. In really, we need to classify the valence states according to the small irreducible representations of $\vec{k}$ - group at the specific $\vec{k}$ - point. Therefore, the admissible symmetries for the first removal

state can be very different with regard for the nature of the partial contribution to the total spectral intensity and $\vec{k}$ - point symmetry. The generalized tight binding (GTB-) approach [4] represents an interesting opportunity to investigate the reasons resulting in the matrix element effects in ARPES- spectrum from above wider view.

Analyzing ARPES-data from the oxychlorides we deal with a charge-transfer insulator [5] and the appropriate low-energy model is reduced to the one-band Habbard model or extended $t - J$-model only in the special case [4]. In this case there is the nondegenerate ground singlet state. In HTSCs, as believe, the ground state is the ZR-state. The last statement has basically the experimental character [1, 2]. In contrast, the theoretical investigations don't give the unequivocal conclusion about a nature of the ground state in HTSCs. In the ab-initio works [6] it was find that ZR-state competes with $^3B_{1g}$ - triplet state, especially, in the area of the doped HTSC-sructures. The calculations show the triplet level is situated on $0.5 - 1eV$ above A_{1g} - level [4, 7]. Moreover there is a crossover between the singlet and triplet levels at some parameters of the calculations. The above magnitudes are approximately equal to a width of the valence bands in HTSCs and we think, that there is a problem to coordinate theoretical and recent experimental conclusions.

In the works [4, 8] we have calculated the dispersion, spectral intensity and parity of quasiparticle states along the high symmetric directions of BZ, within the frameworks d_x , d_z , p_x/p_y , p_z - five orbital general tight binding (GTB-) approach. The calculations reproduce the partial contributions from out-of-plane states: d_z and p_z in Γ - and M - symmetric points of BZ, due to a crossing and hybridization of the bands of ZR- and $^3B_{1g}$ - valence states. It is surprising, that, with regard for the magnitudes of partial contributions, a calculated picture of the spectral intensity and its dependence on the polarization also are coordinated with observed ones [8].

In present work we reproduce the partial contributions from the in-plane and out-of-plane states to the total spectral intensity on all BZ and give a probable interpretation for the remnant FS in the oxychlorides as $\vec{k}$ -area for the in-plane contribution only. As well known, ZR- states are A_{1g} - symmetrized combination of $3d_x$, $2p_x/2p_y$- in-plane orbitales and, in turn, the triplet states are $^3B_{1g}$ - symmetrized combination of $3(2)p_z$, $3d_z$, - out-of-plane orbitales on the whole. Let's notice also, that the partial contribution from $2p_x/2p_y$ - in-plane orbitales to $^3B_{1g}$ - triplet states is not zero but is small in the all BZ [8]. We believed that in $\overrightarrow{k}$ -area for the basic contribution from the out-of-plane states the dependence of

the spectral intensity on the photon energy will arise due to the possible three-dimensional effects (3D) (i.e. a monotonic k_z -dependence). And in $\vec{k}$ - area for the basic contribution from the in-plane states the oscillations of spectral intensity at the different photon energies are possible only [2]. The oscillations are caused by the diffraction of an photoelectronic wave on the periodic structure of oxychlorides along c-axis. Namely in this mean we have used the term: " effective dimension" placed in a title of the work.

We will start from the recent results obtained at $T = 0K$ within the framework of GTB-approach where alongside with A_{1g} -state there is the $^3B_{1g}$ - state in the two-hole sector of Gilbert space. They may are briefly summarized as the following:

- on the top of the valence band of oxychlorides in the antiferromagnetic (AFM-) phase there is the pseudogap of the magnetic nature: $E_S\left(\overrightarrow{k}\right) \sim 0 \div 0.4eV$ between the virtual level and valence band. The pseudogap converts into zero at $\vec{k} = \bar{M}$. The virtual level has the small spectral intensity, proportional to the concentration of the zero spin fluctuations n_0. The pseudogap disappears in the paramagnetic (PM-) phase, where the dispersion of the valence band is similar to the dispersion of the optimally and overdoped HTSCs [9];

- the valence band of the oxychlorides has no only two-dimensional character, and on BZ there are the $\vec{k}$ - areas where the triplet contribution from d_z - orbital of copper and p_z - orbital of the apical ions Cl or O isn't precisely equal to zero;

- the experimental k-dependences of QP-amplitude in the spectral intensity of oxichlorides[9] are satisfactorily described by the $\vec{k}$ - dependences of the partial contribution to the total spectral density obtained in the framework of GTB- approach. The feature of these dependencies is the nonzero contribution from triplet states in Γ - and M - symmetric points of BZ.

Thus, the presence of states with the symmetry of distinct from A_{1g} - symmetry, namely of triplet $^3B_{1g}$ - states, does not contradict the ARPES-data. Further we, with a help of the similar approach, will reproduce separately both the $A_{out}(k, E)$ -contribution from the triplet out-of-plane states, and $A_{in}(k, E)$ -contribution from the singlet in-plane states on all BZ. The details of GTB-approach and magnitudes of parameters can be found in the works [4, 10, 11]. The calculation was carried out in AFM- and PM- phases at T=0K. In Fig.1,2(a,b,c) the amplitudes of the quasiparticle peak for the partial contributions: $A_{in}(k, E)$ and $A_{out}(k, E)$ to the total spectral intensity are showed. In Fig.1(d) the dispersion of the quasiparticle peak on all BZ is showed and well reproduces one observed in [9]. In PM-phase (Fig.2(d))
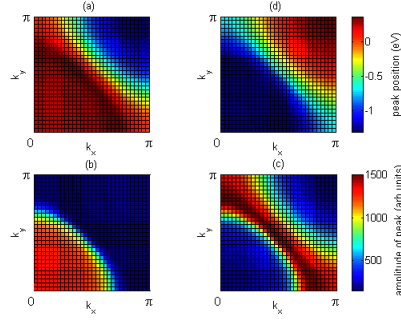
the dispersion is similar to one in doped HTSCs. We have found, that $A_{in}(k, E)$ - partial
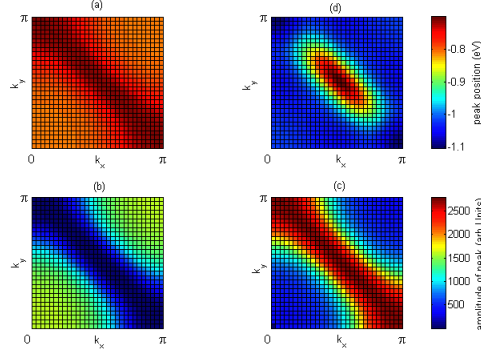

contribution is distributed along $\vec{k}$ - contour close to the edge of the antiferromagnetic BZ (Fig.1(c)) in AFM-phase. In PM-phase (Fig.2(c)), $\vec{k}$ - contour loses the symmetry and to become more close to one of the remnant FS [1]. We can suppose that it is not simple coincidence provided that the procedure of recovery of FS by integration on the fixed energy interval is insufficient in the considered case.

Here, both the dispersion, and spectral intensity are calculated without taking into account the any processes of relaxation. There is only the phenomenological damping $\epsilon = 10^{-3}eV$ to obtain a lorentzian form of curve of spectral intensity (Fig.3). Specificity of considered materials is that namely the strongly correlated nature of the quasiparticle states in BZ result in $\vec{k}$ - dependence of the amplitude of QP. However, we think the specific singlet-triplet character of the quasiparticle states means also the two-channel relaxation process.

The calculations of an effective speed of relaxation with the account for the strong cor-

related nature of the quasiparticle states within the framework of the impurity diagram technique [12] show [13], that in according to Matissen's rule $\left(\tau^\sigma_{eff}\right)^{-1} = \frac{u^2_\sigma}{\tau_{in}} + \frac{\alpha_\sigma v^2_\sigma}{\tau_{out}}$ - the speed of relaxation is additive function of the contributions with weights u^2_σ and v^2_σ , a sense of which consists in the probability with which the carrier participates in the scattering on the appropriate potential for in-plane and out-of-plane states. $u^2_\sigma + v^2_\sigma = 1$, and α_σ depends on the specific character of states and reflects a presence of strong correlations renormalizing the hybridization effects of the states. The scattering potentials for these groups of states can be different, because their spatial nature is different also. It may be effects nonstoichiometry along the in-plane and apical positions or fluctuations of the magnetic moment in and between CuO_2 - planes. For example, we can account the nonstoichiometry effects by means of the following arguments. In the $\vec{k}$ - areas for only triplet contribution $v^2_\sigma \approx 1$ and $\tau^\sigma_{eff} \approx \frac{\tau_{out}}{\alpha_\sigma} \sim c_{out}$, where c_{out} - concentration of the scattering centers for carriers in the out-of-plane states. Along the $\vec{k}$ -contour of the remnant FS accordingly $\tau^\sigma_{eff} \approx \tau_{in} \sim c_{in}$. Note also, that at $v^2_\sigma, u^2_\sigma \neq 0$ due to the absence of the scattering in CuO_2 - planes $c_{in} \to 0$ it
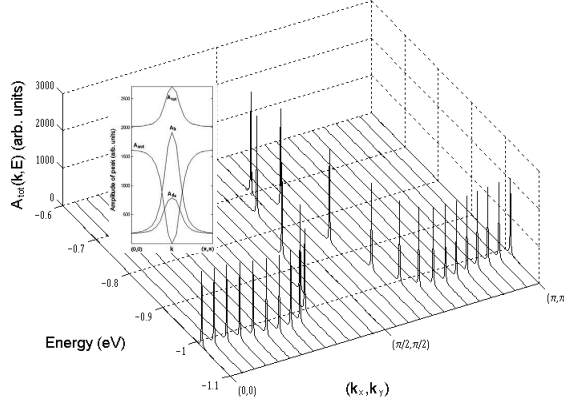
can be obtained $\left(\tau_{eff}^{\sigma}\right)^{-1} \approx \frac{v_{\sigma}^2}{\tau_{out}}$, i.e. the relaxation takes place even at absence of scattering processes in CuO_2 - planes. Thus, crossing from one of $\vec{k}$ - areas BZ in another one we should observe the widening or narrowing of the quasiparticle peak in according to relation between c_{out} and c_{in}. In the case $c_{out} >> c_{in}$ the amplitude of qusiparticle peak in $\vec{k}$ -area for the triplet states falls and to collect all intensity the much greater energy interval than in $\vec{k}$ -area for contribution only from the in-plane states is required.

The two-channel scattering of carriers on the spin fluctuations may be more actual in the oxychlorides. In the experiments using a magnetic neutron scattering, in contrast the classical K_2NiF_4 where a transition to the 3D- Bragg peak observed in 2%- interval from T_N, the dynamic scattering in La_2CuO_4 transformed in the three-dimensional one from $T_N = 195K$ gradually. Even at the high temperatures $\sim 350K$ the low-energy spin fluctuations in $La_{1.89}Sr_{0.11}CuO_4$ have still $3D-$ character [13]. According to empirical conclusions, the lengths of spin correlations are equal to $\xi_{||} \approx 18 \pm 6$Å and $\xi_{\perp} \approx 5.5 \pm 2.2$Å. At the same temperature the carrier in the out-of-plane state from $^3B_{1g}-$ symmetrized combina-

tion, situated at the more hot spot of BZ than the carrier in the in-plane state from $A_{1g}-$ symmetrized combination.

Thus, the method of integration with a constant interval is unacceptable at the presence of contributions to the total spectral intensity from so different states. There is a risk, that the method of the integration used in [1] does not reproduce in particular not only the remnant FS, but also one of the contributions to the total spectral intensity with least relaxation time. Namely the contribution from d_x -, p_x / p_y - orbitales.

We think, that as consequence of the scattering processes, the contribution from the triplet states reproduces, in turn, a noncoherent part of the spectral intensity in ARPES-spectra of oxychlorides. Therefore the effective dimension of the quasiparticle states can rise up to 3D in the vicinity of Γ - and M - symmetric points of BZ. In these $\overrightarrow{k}$ - areas we can expect the monotonic dependence of the noncoherent part on the photon energy. Probably, there is also an opportunity to observe not only oscillations of the coherent part as it was made in work [14], but oscillations of the relation of the coherent and noncoherent parts of the spectral intensity at the different photon energy.

I. CAPTURE OF FIGURES

Fig.1 $\overrightarrow{k}$ - dependence of the: total spectral intensity (a), out-of-plane spectral intensity (b), in-plane spectral intensity (c) and QP position (d) in AFM at $T = 0K$.

Fig.2 $\overrightarrow{k}$ - dependence of the: total spectral intensity (a), out-of-plane spectral intensity (b), in-plane spectral intensity (c) and QP position (d) in PM at $T = 0K$.

Fig.3 3D-view on the quasiparticle peak in the total spectral intensity along $\Gamma \leftrightarrow M$ - direction in AFM, $A_{tot}(\overrightarrow{k}, E) = A_{d_X}(\overrightarrow{k}, E) + A_b(\overrightarrow{k}, E) + A_{out}(\overrightarrow{k}, E)$. The inset shows $\vec{k}$

- dependence of the partial contibutions to an amplitude of QP along $\Gamma \leftrightarrow M$ - direction.

[1] F.Ronning, C.Kim, D.F.Feng, D.S.Marshall, A.G.Loeser, L.L.Miller, J.N.Eckstein, I.Bozovic, Z.X.Shen, Science, **282**, 2067 (1998).

[2] S.Haffner, D.M.Brammeier, C.G.Olson, L.L.Miller, and Lynch, Phys.Rev. B **63**, 212501 (2001).

[3] M.Grioni, H.Berger, S.Larosa, I.Vobornik, F.Zwick, G.Mragaritondo, R.Kelley, J.Ma, M.Onellion, Physica B, **230-232**, 825 (1997).

[4] V.A.Gavrichkov, S.G.Ovchinnikov, A.A.Borisov, and E.G.Goryachev, JETP, **91**, 2, 369 (2000).

[5] J.Zaanen, G.A.Sawatzky, J.W.Allen, Phys.Rev.Lett. **55**, 4128 (1985).

[6] H.Kamimura, M.Eto, J.Phys.Soc.Jpn. **59**, 3053 (1990).

[7] H.Eskes, L.H.Tjeng, G.A.Sawatzky, Phys.Rev. B **41**, 288 (1990).

[8] V.A.Gavrichkov, A.A.Borisov, S.G.Ovchinnikov, Phys.Rev. B **64**, 235124 (2001).

[9] B.O.Wells, Z.-X.Shen, A.Matsuura, et.al., Phys.Rev.Lett.**74**, 964 (1995).

[10] L.F.Feiner, J.H.Jefferson, and R.Raimondi, Phys.Rev. B **53**, 8751 (1996).

[11] L.F.Feiner, J.H.Jefferson, and R.Raimondi, Phys.Rev. B **53**, 8751 (1996).

[12] A.A.Abrikosov, L.P.Gor'kov, I.E.Dzyaloshinski, Methods of quantum field theory in statistic physics, Gostehizdat, M, 350 pp. (1962).

[13] V.A.Gavrichkov, S.G.Ovchinnikov, Fiz.Tverd.Tel. **41**, 68 (1999).

[14] R.J.Birgeneau, G.Shiran, in *Physical properties of High Temperature Superconductors I*, edited by Donald M.Ginsberg (World Scientific, Singapore, 1989), pp.151-211.

[15] C.Durr, S.Legner, R.Hayn, S.V.Borisenko, Z.Hu, A.Theresiak, M.Knupfer, M.S.Golden, and J.Fink, and F.Ronning, Z.-X.Shen, and H.Eisaki, S.Uchida, and C.Janowitz, R.Muller, R.L.Johnson, and K.Rossnagel, L.Kipp, G.Reichardt, Phys.Rev. B **63**, 014505 (2000).